Where the APS could be in 2013 for X-ray Absorption Spectroscopies Matthew Newville, CARS, The University of Chicago 28-July-2008

X-ray absorption spectroscopies (XAS, including EXAFS, XANES, and XMCD) are relatively mature techniques that make use of energy-tunable x-ray sources to study the atomic-scale structure, chemical environment, and magnetic state of selected elements. These techniques do not rely on sample form (for example, crystallinity), and are sensitive to very dilute elemental species in complex systems. These properties make XAS attractive for study of highly disordered systems, including nanoparticles, liquids, molecules, and heterogeneous materials, and so applicable to important research areas for many fields. In addition, the elemental-specificity of XAS is closely related to resonant inelastic x-ray scattering, x-ray Raman spectroscopy, hard x-ray photoemission, and resonant elastic scattering. At the APS, XAS has been coupled successfully to micro-beams, and used extensively for environmental, chemical, and material sciences. Currently, most beamlines at the APS using XAS as a core technique are CAT beamlines or those taken over by XOR after being fully developed and running successful user programs. However, about one-third of the beamline proposals touch a need for improving, upgrading, or enabling new uses of XAS or related spectroscopies that use core-electron level resonances.

There are a few important ways in which the APS could lead development and use of XAS and related techniques.

First, the APS could develop support infrastructure for sample environments, detectors, and data analysis and interpretation specific to XAS. Examples of these infrastructures are

- facilities to modify high-pressure diamond anvils suitable for low-energies (6-10keV) -- drilled diamonds, and for poly-crystalline anvils to avoid inevitable Bragg peaks from the diamond anvils.
- gas-handling systems for in situ and in operando catalysis work.
- an active Theory group and Analysis Software group that focused on some of the imperfect aspects of XAS Theory and Analysis.

Second, while XAS at the APS is quite strong in micro-XAFS and applications in environmental science, the APS could work to expand support for important applications of XAS that are underrepresented at the APS (relative to how XAS is used at other facilities), especially catalysis and life sciences. There is currently no dedicated facilities at the APS for XAS in either of these two important fields.

Third, the APS could more fully support the development of better detector systems for XAS. Detector needs for XAS are primarily for fluorescence XAS, which are currently led by Si-drift fluorescence detectors. With multi-element Si-drift and Ge-drift fluorescence detectors, the APS XAS community could gain an order of magnitude in count rate and sensitivity.

The most efficient approach that the APS could take would be to follow the work of Siddons and Ryan at BNL/ASRP on the so-called 'Maya' detector.

But probably the biggest impact on XAS that the APS could take would be to lead in the development of RIXS / high-resolution fluorescence for more wide-spread application in areas currently using XAS. This technique (measuring the K-edge EXAFS decaying into a ~1eV bandwidth of a specific alpha or beta fluorescence line) has been proven to be able to add two new "knobs" on XAS: spin-selectivity, and species-selectivity, both of which have very high potential for applications in existing areas and expanding our abilities to study new problems. While these techniques are demonstrated, they generally need sources with high brightness, and there are few beamlines in the world dedicated to these advanced techniques. With a fairly small effort, the APS could become the leader in the application of these techniques as an improvement over current XAS measurements.

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